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TITLE : AGENT FOR IMPARTING  
 IRIDESCENT LUSTER TO COSMETIC



ABSTRACT : PURPOSE: To provide an agent for imparting excellent iridescent luster to cosmetics, and keeping the luster stably for a long period even at a high temperature, by using a straight-chain alkanediol diester as a main component.  
 CONSTITUTION: The objective iridescent luster agent contains at least one compound of formula (R and R' are 13-23C straight-chain alkyl; n is integer 3-10) pref. having a melting point of  $\geq 50$  deg.C. The agent gives very beautiful and thermally stable iridescent luster to liquid or pasty cosmetics such as shampoo, rinsing agent, lotion, cream, etc., by conventional compounding process. The use of a mixture of two or more kinds of the above compounds or the use of a compound wherein R is different from R' gives more desirable iridescent luster than the use of a compound wherein R is R'. Since larger molecular weight of R and R' results in higher melting point of the compound, desired thermal stability according to the purpose can be attained by selecting proper R and R'.

78186-34-2 9,10-Anthracenedicarboxaldehyde, bis[4,5-dihydro-1H-imidazol-2-yl]hydrazonol  
C<sub>22</sub>H<sub>12</sub>N<sub>4</sub>

78186-35-3 Iodine chloride (ICl<sub>3</sub>) C<sub>1</sub>I<sub>3</sub>

78186-36-4 Propanoic acid, 2-methyl-, (2S)-phenyl-1,2,4-triazin-3-ylhydrazide, hydrochloride C<sub>13</sub>H<sub>15</sub>N<sub>5</sub>O<sub>3</sub>·ClH

78186-37-5 4-Piperidinecarboxamide, N-(2,6-dimethylphenyl)-1-methyl-, monohydrochloride C<sub>15</sub>H<sub>21</sub>N<sub>3</sub>O·ClH

78186-38-6 Benzenemethanamine, 2,5-dimethoxy- $\alpha$ , $\alpha$ -dimethyl-, C<sub>11</sub>H<sub>17</sub>N<sub>2</sub>O<sub>2</sub>

78186-39-7 Isoquinolinium, 2-[3-(4-[(hydroxyimino)methyl]pyridinyl)propyl]-, dibromide C<sub>15</sub>H<sub>19</sub>N<sub>3</sub>O<sub>2</sub>Br<sub>2</sub>

78186-40-0 Methanesulfonamide, N-[4-(9-acridinylamino)-3-methoxyphenyl]-, methanesulfonate C<sub>21</sub>H<sub>19</sub>N<sub>3</sub>O<sub>5</sub>·CH<sub>3</sub>SO<sub>3</sub>S

78186-41-1 Methanesulfonamide, N-[4-(9-acridinylamino)phenyl]-, hydrochloride C<sub>21</sub>H<sub>19</sub>N<sub>3</sub>O<sub>3</sub>·ClH

78186-42-2 Morpholinium, 4,4'-[1,1'-biphenyl-1,4'-diylbis(2-oxo-2,1-ethenediyl)]bis[4-ethyl-, dibromide C<sub>24</sub>H<sub>28</sub>N<sub>2</sub>O<sub>4</sub>Br<sub>2</sub>

78186-43-3 Morpholine, 4-[2-(2-methyl-2-naphthyl-2,3-dioxol-2-yl)ethoxy]-ethyl-, 2-hydroxy-1,2,3-propanetricarboxylate C<sub>20</sub>H<sub>25</sub>N<sub>3</sub>O<sub>8</sub>·xH<sub>2</sub>O

78186-44-4 Benzenemethanol,  $\alpha$ -(2-(diethylamino)-1-methylethyl)-3-fluoro- $\alpha$ -(3-fluorophenyl)-, hydrobromide C<sub>20</sub>H<sub>25</sub>F<sub>2</sub>N<sub>2</sub>O·BrH

78186-45-5 Benzenemethanol,  $\alpha$ -(2-(diethylamino)-1-methylethyl)-4-methyl- $\alpha$ -(4-methylphenyl)-, hydrochloride C<sub>22</sub>H<sub>29</sub>N<sub>2</sub>O·ClH

78186-46-6 Benzenemethanol,  $\alpha$ -(2-(diethylamino)-1-methylethyl)- $\alpha$ -(3,4-dimethoxyphenyl)-3,4-dimethoxy-, C<sub>24</sub>H<sub>31</sub>N<sub>2</sub>O<sub>4</sub>

78186-47-7 Benzenemethanol,  $\alpha$ -(2-[(2-(dimethylamino)ethyl)methylamino]-1-methylethyl)- $\alpha$ -phenyl-, dihydrochloride C<sub>21</sub>H<sub>29</sub>N<sub>3</sub>O<sub>2</sub>·2ClH

78186-48-8 Benzenemethanol,  $\alpha$ -(2-[(2-furanylmethyl)amino]-1-methylethyl)- $\alpha$ -phenyl-, C<sub>21</sub>H<sub>27</sub>N<sub>2</sub>O<sub>2</sub>

78186-49-9 Benzenemethanol,  $\alpha$ -(2-[(2-furanylmethyl)amino]-1-methylethyl)- $\alpha$ -phenyl-, (Z)-2-butenedioate (salt) C<sub>21</sub>H<sub>27</sub>N<sub>2</sub>O<sub>4</sub>·C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>

78186-50-2 Benzenemethanol,  $\alpha$ -(2-[(2-furanylmethylene)amino]-1-methylethyl)- $\alpha$ -phenyl-, C<sub>21</sub>H<sub>27</sub>N<sub>2</sub>O<sub>2</sub>

78186-51-3 Benzenemethanol,  $\alpha$ -(2-(methylamino)propyl)- $\alpha$ -phenyl-, hydrochloride C<sub>17</sub>H<sub>21</sub>N<sub>2</sub>O·ClH

78186-52-4 Benzenemethanol,  $\alpha$ -(1-methyl-2-[(1-methyl-4-piperidinylamino)ethyl]- $\alpha$ -phenyl-, dihydrochloride C<sub>24</sub>H<sub>35</sub>N<sub>3</sub>O<sub>2</sub>·2ClH

78186-53-5 Benzenemethanol,  $\alpha$ -(1-methyl-2-(propylamino)ethyl)- $\alpha$ -phenyl-, (Z)-2-butenedioate (salt) C<sub>19</sub>H<sub>25</sub>N<sub>2</sub>O<sub>4</sub>·C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>

78186-54-6 Benzenecetic acid,  $\alpha$ -hydroxy- $\alpha$ -phenyl-, 3-(dibutylamino)propyl ester C<sub>23</sub>H<sub>33</sub>N<sub>2</sub>O<sub>3</sub>

78186-55-7 1,3-Benzodioxol-5-amine, 2-methyl-2-[2-(4-morpholinyl)ethyl]-, dihydrochloride, hemihydrate C<sub>18</sub>H<sub>23</sub>N<sub>3</sub>O<sub>5</sub>·2ClH<sub>2</sub>·1/2H<sub>2</sub>O

78186-56-8 1,2-Ethanediamine, N,N-diethyl-, N-(1-methyl-2-(2-methyl-1,3-benzodioxol-2-yl)ethyl)-, C<sub>17</sub>H<sub>27</sub>N<sub>2</sub>O<sub>2</sub>

78186-57-9 1,2-Ethanediamine, N,N-diethyl-, N-(1-methyl-2-(2-methyl-1,3-benzodioxol-2-yl)ethyl)-, (Z)-2-butenedioate (1:2) C<sub>17</sub>H<sub>27</sub>N<sub>2</sub>O<sub>4</sub>·C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>

78186-58-9 Ethanediamine, N,N-diethyl-, 2-methyl-1,3-benzodioxol-2-yl-[(2-methyl-1,3-benzodioxol-2-yl)ethyl]thio-, 2-hydroxy-1,2,3-propanetricarboxylate C<sub>18</sub>H<sub>23</sub>N<sub>2</sub>O<sub>8</sub>·xH<sub>2</sub>O

78186-59-1 1-Propanamine, N,N-diethyl-3-[2-(2-methyl-1,3-benzodioxol-2-yl)ethoxy]-, 2-hydroxy-1,2,3-propanetricarboxylate C<sub>17</sub>H<sub>27</sub>N<sub>2</sub>O<sub>8</sub>·xH<sub>2</sub>O

78186-60-4 1,3-Benzodioxole-5,6-dimethanol C<sub>10</sub>H<sub>10</sub>O<sub>4</sub>

78186-61-5 1,3-Benzodioxol-2-amine, N,2-dimethyl-, hydrochloride C<sub>9</sub>H<sub>11</sub>N<sub>2</sub>O<sub>2</sub>·ClH

78186-62-6 Piperazine, 1-methyl-4-(2-methyl-1,3-benzodioxol-2-yl)ethyl-, hydrochloride C<sub>15</sub>H<sub>23</sub>N<sub>2</sub>O<sub>2</sub>·ClH

78186-63-7 Piperidine, 1-[2-methyl-2-(2-(1-piperidinyl)ethyl)-1,3-benzodioxol-5-yl]methyl-, dihydrochloride, hemihydrate C<sub>21</sub>H<sub>29</sub>N<sub>3</sub>O<sub>2</sub>·2ClH<sub>2</sub>·1/2H<sub>2</sub>O

78186-64-8 Piperidine, 1-[3-(2-(2-methyl-1,3-benzodioxol-2-yl)ethoxy)propyl]-, hydrobromide C<sub>18</sub>H<sub>27</sub>N<sub>2</sub>O<sub>2</sub>·BrH

78186-65-9 26,12-(Epoxyethano)-12H-benzofuro[4',3':2,8,10]dibenzol[8',9',10',11']-[1,6]-dioxacyclododecino[3',2',3']-[2,6]benzodioxacyclo-undecino[11,12-b]quinoxaline C<sub>28</sub>H<sub>28</sub>N<sub>2</sub>O<sub>6</sub>

78186-66-0 Prost-13-ene-1,9-dione, 11,16-dihydroxy-1-(hydroxymethyl)-16-(1-propynyl)-, (11 $\alpha$ ,13 $\alpha$ ,15 $\alpha$ ) C<sub>24</sub>H<sub>38</sub>O<sub>5</sub>

78186-67-1 Prost-13-en-1-ol, 11-(acetoxy)-5-bromo-6,9-epoxy-15-hydroxy-15-phenyl-, methyl ester, (6S,9 $\alpha$ ,11 $\alpha$ ,13 $\alpha$ ,15S) C<sub>28</sub>H<sub>38</sub>BrO<sub>6</sub>

78186-68-2 Prost-13-en-1-ol, 11-(acetoxy)-5-bromo-6,9-epoxy-15-hydroxy-15-phenyl-, methyl ester, (6S,9 $\alpha$ ,11 $\alpha$ ,13 $\alpha$ ,15R) C<sub>28</sub>H<sub>38</sub>BrO<sub>6</sub>

78186-69-3 2H-Cyclopenta[b]furan-2-pentanoic acid, 4-formylhexahydro- $\delta$ -iodo-, methyl ester C<sub>14</sub>H<sub>21</sub>IO<sub>4</sub>

78186-70-6 Cyclopenta[b]pyran-2-butanolic acid, 5-(4-butoxy-4-methyl-3-oxo-1-pentenyl)-octahydro-6-hydroxy-, methyl ester, [2S-(2a,4aa,5a(E),6b,7aa)] C<sub>24</sub>H<sub>38</sub>O<sub>6</sub>

78186-71-7 Prost-13-en-1-ol, 11-(acetoxy)-5,9-epoxy-15-methoxy-16-methyl-, methyl ester, (5R,9 $\alpha$ ,11 $\alpha$ ,13 $\alpha$ ,15S,16S) C<sub>28</sub>H<sub>42</sub>O<sub>6</sub>

78186-72-8 Prost-13-en-1-ol, 11-(acetoxy)-5,9-epoxy-15-methoxy-16-methyl-, methyl ester, (5R,9 $\alpha$ ,11 $\alpha$ ,13 $\alpha$ ,15R,16S) C<sub>28</sub>H<sub>42</sub>O<sub>6</sub>

78186-73-9 Prost-13-en-1-ol, 5,9-epoxy-15-ethynyl-11,15-dihydroxy-, (5S,9 $\alpha$ ,11 $\alpha$ ,13 $\alpha$ ,15R) C<sub>27</sub>H<sub>40</sub>O<sub>4</sub>

78186-74-0 Prost-13-yn-1-ol, 6,9-epoxy-15-methoxy-, (6R,9 $\alpha$ ) C<sub>21</sub>H<sub>34</sub>O<sub>4</sub>

78186-75-1 Prost-13-yn-1-ol, 6,9-epoxy-15-methoxy-, (6S,9 $\alpha$ ) C<sub>21</sub>H<sub>34</sub>O<sub>4</sub>

78186-76-2 Prost-13-yn-1-ol, 6,9-epoxy-15-ethoxy-15-hydroxy-16-methyl-, ethyl ester, (6R,9 $\alpha$ ,11 $\alpha$ ,15S,16S) C<sub>28</sub>H<sub>42</sub>O<sub>6</sub>

78186-77-3 Iron, hexacarbonyl[ $\mu$ -(1 $\eta^5$ - $\eta^1$ -(3,7,8-tris(methylene)bicyclo[2.2.2]oct-5-en-2-ylidene)-2-propanone)]di-, stereoisomer C<sub>18</sub>H<sub>14</sub>FeO<sub>7</sub>

78186-78-4 2H-Pyranol[2',3':4',5']benzofuro[2',3':4']cyclobuta[1,2-d]pyrimidine-2,8,10(7bH,9H)-trione, 7a,11,11a,11b-tetrahydro-4,7a,7b-trimethyl-, C<sub>24</sub>H<sub>28</sub>N<sub>2</sub>O<sub>3</sub>

78186-79-5 2H-Pyranol[2',3':4',5']benzofuro[3',2':3,4]cyclobuta[1,2-d]pyrimidine-2,9,11(7aH,10H)-trione, 7b,8,11a,11b-tetrahydro-4,7a,11a-trimethyl-, C<sub>24</sub>H<sub>28</sub>N<sub>2</sub>O<sub>3</sub>

78186-80-8 5-Hexen-3-one, 4,4-dimethyl-, C<sub>10</sub>H<sub>18</sub>O

78186-81-9 5-Hexen-3-one, 1-ethoxy-, C<sub>11</sub>H<sub>20</sub>O<sub>2</sub>

78186-82-0 Carbonotrithioic acid, 1,2-ethanediy ester, dilithium salt C<sub>2</sub>H<sub>6</sub>S<sub>2</sub>Li<sub>2</sub>

78186-83-1 Carbonotrithioic acid, 2-(1,3-dithiolan-2-ylthio)ethyl methyl ester C<sub>7</sub>H<sub>12</sub>S<sub>2</sub>

78186-84-2 Carbonotrithioic acid, 1,2-ethanediy bis(phenylmethyl) ester C<sub>18</sub>H<sub>16</sub>S<sub>2</sub>

78186-85-3 1,3-Dithiolane-2-thione, 4-ethyl-, C<sub>6</sub>H<sub>8</sub>S<sub>2</sub>

78186-86-4 Carbonotrithioic acid, butyl 2-(1,3-dithiolan-2-ylthio)ethyl ester C<sub>10</sub>H<sub>18</sub>S<sub>2</sub>

78186-87-5 Carbonotrithioic acid, 2-(1,3-dithiolan-2-ylthio)ethyl ethyl ester C<sub>11</sub>H<sub>18</sub>S<sub>2</sub>

78186-88-6 Carbonotrithioic acid, 1,2-ethanediy dipropyl ester C<sub>10</sub>H<sub>16</sub>S<sub>2</sub>

78186-89-7 Carbonotrithioic acid, 2-(1,3-dithiolan-2-ylthio)ethyl propyl ester C<sub>11</sub>H<sub>18</sub>S<sub>2</sub>

78186-90-0 Carbonotrithioic acid, 1,2-ethanediy dibutyl ester C<sub>12</sub>H<sub>20</sub>S<sub>2</sub>

78186-91-1 Acetic acid, (dimethoxyphosphinyl)-hydroxy-, methyl ester C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>P

78186-92-2 Acetic acid, (dimethoxyphosphinyl)-2-(ethoxyethoxy)-, methyl ester C<sub>8</sub>H<sub>16</sub>O<sub>7</sub>P

78186-93-3 Acetic acid, (dimethoxyphosphinyl)-[(tetrahydro-2H-pyran-2-yl)oxy]-, methyl ester C<sub>10</sub>H<sub>18</sub>O<sub>7</sub>P

78186-94-4 Acetic acid, (dimethoxyphosphinyl)-1-methoxy-1-methylethoxy-, methyl ester C<sub>8</sub>H<sub>16</sub>O<sub>7</sub>P

78186-95-5 Acetic acid, (dimethoxyphosphinyl)-[(1,1-dimethylethyl)dimethylsilyloxy]-, methyl ester C<sub>11</sub>H<sub>22</sub>O<sub>6</sub>PSi

78186-96-6 2-Pentenoic acid, 4-methyl-2-[(tetrahydro-2H-pyran-2-yl)oxy]-, methyl ester, (Z) C<sub>12</sub>H<sub>20</sub>O<sub>3</sub>

78186-97-7 2-Pentenoic acid, 2-[(1,1-dimethylethyl)dimethylsilyloxy]-4-methyl-, methyl ester, (E) C<sub>13</sub>H<sub>24</sub>O<sub>3</sub>Si

78186-98-8 2-Hexenoic acid, 2-(2-ethoxyethoxy)-5-methyl-, methyl ester, (E) C<sub>12</sub>H<sub>22</sub>O<sub>4</sub>

78186-99-9 2-Hexenoic acid, 2-(1-methoxy-1-methylethoxy)-5-methyl-, methyl ester, (E) C<sub>12</sub>H<sub>22</sub>O<sub>4</sub>

78187-00-5 1H-Pyrrole-1-carboxylic acid, 3-(2-ethoxyethoxy)-2,5-dihydro-2-oxo-5-(phenylmethyl)-, phenylmethyl ester, (±) C<sub>22</sub>H<sub>25</sub>N<sub>2</sub>O<sub>4</sub>

78187-01-6 2-Pentenoic acid, 2-(2-ethoxyethoxy)-5-phenyl-4-[(phenylmethoxy)carbonyl]amino-, methyl ester, (±) C<sub>25</sub>H<sub>31</sub>N<sub>2</sub>O<sub>5</sub>

78187-02-7 2H-Pyrrrol-2-one, 3-(2-ethoxyethoxy)-5,5-dihydro-5-(phenylmethyl)-, (±) C<sub>15</sub>H<sub>19</sub>N<sub>2</sub>O<sub>3</sub>

78187-03-8 2H-Pyrrrol-2-one, 1-acetyl-1,5-dihydro-3-hydroxy-5-(phenylmethyl)-, (±) C<sub>15</sub>H<sub>19</sub>N<sub>2</sub>O<sub>3</sub>

78187-04-9 2-Pentenoic acid, 4-methyl-2-[(tetrahydro-2H-pyran-2-yl)oxy]-, methyl ester, (Z) C<sub>12</sub>H<sub>20</sub>O<sub>4</sub>

78187-05-0 2-Pentenoic acid, 2-[(1,1-dimethylethyl)dimethylsilyloxy]-4-methyl-, methyl ester, (Z) C<sub>13</sub>H<sub>24</sub>O<sub>3</sub>Si

78187-06-1 2-Hexenoic acid, 2-(2-ethoxyethoxy)-5-methyl-, methyl ester, (Z) C<sub>12</sub>H<sub>22</sub>O<sub>4</sub>

78187-07-2 2-Hexenoic acid, 2-(1-methoxy-1-methylethoxy)-5-methyl-, methyl ester, (Z) C<sub>12</sub>H<sub>22</sub>O<sub>4</sub>

78187-08-3 Oxiranecarboximidothioic acid, 3-(2-chlorophenyl)-2-cyano-, propyl ester C<sub>13</sub>H<sub>13</sub>ClN<sub>2</sub>OS

78187-09-4 Oxiranecarboximidic acid, 3-(2-chlorophenyl)-2-cyano-, methyl ester C<sub>11</sub>H<sub>11</sub>ClN<sub>2</sub>O<sub>2</sub>

78187-10-7 2,2-Oxiranedicarboximidic acid, 3-(2-chlorophenyl)-, dimethyl ester C<sub>12</sub>H<sub>13</sub>ClN<sub>2</sub>O<sub>3</sub>

78187-11-8 Oxiranecarboxamide, 3-(2-chlorophenyl)-2-cyano-, trans-C<sub>10</sub>H<sub>9</sub>ClN<sub>2</sub>O<sub>2</sub>

78187-12-9 Oxiranecarboxamide, 3-(2-chlorophenyl)-2-cyano-, cis-C<sub>10</sub>H<sub>9</sub>ClN<sub>2</sub>O<sub>2</sub>

78187-13-0 Oxiranecarboxamide, 3-(2-chlorophenyl)-2-cyano-N-(2-(2-hydroxyethoxy)methyl)-, trans-C<sub>14</sub>H<sub>15</sub>ClN<sub>2</sub>O<sub>4</sub>

78187-14-1 1,3,2-Dithiaphospholane, 2-(1,1-dimethylethyl)-, 2-oxide C<sub>6</sub>H<sub>10</sub>OPS<sub>2</sub>

78187-15-2 1,3,2-Dithiaphospholane, 2-(1,1-dimethylethyl)-, 2-sulfide C<sub>6</sub>H<sub>10</sub>PS<sub>3</sub>

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78187-16-3 1,3,7,9-Tetrathia-2,8-diphosphacyclododecane, 2,8-dimethyl-, 2,8-disulfide, stereoisomer C<sub>14</sub>H<sub>18</sub>P<sub>2</sub>S<sub>6</sub>

78187-17-4 Phosphonodithioic acid, (1,1-dimethylethyl)-, diethyl ester C<sub>8</sub>H<sub>14</sub>P<sub>2</sub>S<sub>2</sub>

78187-18-5 Benzene, 1,1'-(1,2-ethanediy)bis-(oxy-2,1-ethanediyloxy)bis[4-methyl-2-nitro-C<sub>6</sub>H<sub>4</sub>N<sub>2</sub>O<sub>2</sub>]

78187-19-6 Benzenamine, 2,2'-(1,2-ethanediy)bis-(oxy-2,1-ethanediyloxy)bis[5-methyl-C<sub>6</sub>H<sub>4</sub>N<sub>2</sub>O<sub>2</sub>]

78187-20-9 Dodecanoic acid, 5-(nitrosooxy)-, potassium salt C<sub>12</sub>H<sub>23</sub>NO<sub>4</sub>K

78187-21-0 Dodecanoic acid, 7-(nitrosooxy)-, potassium salt C<sub>12</sub>H<sub>23</sub>NO<sub>4</sub>K

78187-22-1 Dodecanoic acid, 8-(nitrosooxy)-, potassium salt C<sub>12</sub>H<sub>23</sub>NO<sub>4</sub>K

78187-23-2 Dodecanoic acid, 10-(nitrosooxy)-, potassium salt C<sub>12</sub>H<sub>23</sub>NO<sub>4</sub>K

78187-24-3 Dodecanoic acid, 12-(nitrosooxy)-, potassium salt C<sub>12</sub>H<sub>23</sub>NO<sub>4</sub>K

78187-25-4 Dodecanoic acid, 6-oxo-, potassium salt C<sub>12</sub>H<sub>23</sub>O<sub>3</sub>K

78187-26-5 Dodecanoic acid, 7-oxo-, potassium salt C<sub>12</sub>H<sub>23</sub>O<sub>3</sub>K

78187-27-6 Propanedioic acid, [3-acetyl-6-(1,1-dimethylethyl)-2-cyclohexen-1-yl]-, diethyl ester, cis-C<sub>18</sub>H<sub>30</sub>O<sub>5</sub>

78187-28-7 Ethanone-2,2-ds, 1-[4-(1,1-dimethylethyl)-1-cyclohexen-1-yl]- C<sub>12</sub>H<sub>18</sub>D<sub>2</sub>O

78187-29-8 Ethanone-2,2-ds, 1-[4-(1,1-dimethylethyl)-1-cyclohexen-1-yl-3-d], trans-C<sub>12</sub>H<sub>18</sub>D<sub>2</sub>O

78187-30-1 Ethanone-2,2-ds, 1-[4-(1,1-dimethylethyl)-1-cyclohexen-1-yl-3-ds]- C<sub>12</sub>H<sub>18</sub>D<sub>2</sub>O

78187-31-2 2-Cyclohexene-1-acetic acid, 3-acetyl- $\alpha$ -cyano-6-(1,1-dimethylethyl)-, ethyl ester C<sub>17</sub>H<sub>28</sub>NO<sub>3</sub>

78187-32-3 Pentyl, 1-mercapto-1,3-dimethyl-, C<sub>7</sub>H<sub>15</sub>S

78187-33-4 Sulfur, (1,1-dimethylethyl)(1,3-dimethylpentyl)hydro- C<sub>11</sub>H<sub>22</sub>S

78187-34-5 Sulfur, bis(1,1-dimethylethyl)hydrodi-C<sub>6</sub>H<sub>14</sub>S<sub>2</sub>

78187-35-6 Pyrrolidine, 1,3-dimethyl-3-(1-methylethyl)-2-(3,4,5-trimethoxyphenyl)-, cis-C<sub>18</sub>H<sub>27</sub>NO<sub>3</sub>

78187-36-7 Pyrrolidine, 2-(4-chlorophenyl)-1,3-dimethyl-3-(1-methylethyl)-, cis-C<sub>18</sub>H<sub>27</sub>ClN

78187-37-8 Pyrrolidine, 1,3-dimethyl-3-(1-methylethyl)-2-(3,4,5-trimethoxyphenyl)-, hydrochloride, cis-C<sub>18</sub>H<sub>27</sub>NO<sub>3</sub>·ClH

78187-38-9 Pyrrolidine, 2-(4-chlorophenyl)-1,3-dimethyl-3-(1-methylethyl)-, hydrochloride, cis-C<sub>18</sub>H<sub>27</sub>ClN·ClH

78187-39-0 Pyrrolidine, 1,3-dimethyl-3-(1-methylethyl)-2-(3,4,5-trimethoxyphenyl)-, cis-C<sub>18</sub>H<sub>27</sub>NO<sub>3</sub>

78187-40-3 Pyrrolidine, 1,3-dimethyl-3-(1-methylethyl)-2-(3,4,5-trimethoxyphenyl)-, hydrochloride, cis-C<sub>18</sub>H<sub>27</sub>NO<sub>3</sub>·ClH

78187-41-4 Pyrrolidine, 1,3-dimethyl-3-(1-methylethyl)-2-phenyl-, cis-C<sub>18</sub>H<sub>27</sub>N

78187-42-5 Pyrrolidine, 1,3-dimethyl-3-(1-methylethyl)-2-phenyl-, hydrochloride, cis-C<sub>18</sub>H<sub>27</sub>N·ClH

78187-43-6 Piperidine, 1,3,3,4-tetramethyl-2-(3,4,5-trimethoxyphenyl)-, cis-C<sub>18</sub>H<sub>27</sub>NO<sub>3</sub>

78187-44-7 Piperidine, 1,3,3,4-tetramethyl-2-(3,4,5-trimethoxyphenyl)-, hydrochloride, cis-C<sub>18</sub>H<sub>27</sub>NO<sub>3</sub>·ClH

78187-45-8 Piperidine, 1,3,3,4-tetramethyl-2-phenyl-, cis-C<sub>18</sub>H<sub>27</sub>N

78187-46-9 Piperidine, 1,3,3,4-tetramethyl-2-phenyl-, hydrochloride, cis-C<sub>18</sub>H<sub>27</sub>N·ClH

78187-47-0 9-Octadecenoic acid (Z)-, 3-[(1-oxotetradecyl)oxy]propyl ester C<sub>25</sub>H<sub>46</sub>O<sub>4</sub>

78187-48-1 9-Octadecenoic acid (Z)-, 3-[(1-oxohexadecyl)oxy]propyl ester C<sub>27</sub>H<sub>50</sub>O<sub>4</sub>

78187-49-2  $\beta$ -D-Glucopyranosiduronic acid, 1,4-dihydro-4-oxo-2-pyrimidinyl 1-thio-, methyl ester, 2,3,4-triacetate C<sub>17</sub>H<sub>25</sub>NO<sub>10</sub>S

78187-50-5  $\beta$ -D-Glucopyranosiduronic acid, 5-chloro-1,4-dihydro-4-oxo-2-pyrimidinyl 1-thio-, methyl ester, 2,3,4-triacetate C<sub>17</sub>H<sub>23</sub>ClN<sub>2</sub>O<sub>10</sub>S

78187-51-6  $\beta$ -D-Glucopyranosiduronic acid, 5-bromo-1,4-dihydro-4-oxo-2-pyrimidinyl 1-thio-, methyl ester, 2,3,4-triacetate C<sub>17</sub>H<sub>23</sub>BrN<sub>2</sub>O<sub>10</sub>S

78187-52-7  $\beta$ -D-Glucopyranosiduronic acid, 1,4-dihydro-6-iodo-4-oxo-2-pyrimidinyl 1-thio-, methyl ester, 2,3,4-triacetate C<sub>17</sub>H<sub>23</sub>IO<sub>10</sub>S

78187-53-8  $\beta$ -D-Glucopyranosiduronic acid, 1,4-dihydro-4-oxo-2-pyrimidinyl 1-thio-, methyl ester C<sub>17</sub>H<sub>25</sub>NO<sub>10</sub>S

78187-54-9  $\beta$ -D-Glucopyranosiduronic acid, 5-chloro-1,4-dihydro-4-oxo-2-pyrimidinyl 1-thio-, methyl ester C<sub>17</sub>H<sub>23</sub>ClN<sub>2</sub>O<sub>10</sub>S

78187-55-0  $\beta$ -D-Glucopyranosiduronic acid, 5-bromo-1,4-dihydro-4-oxo-2-pyrimidinyl 1-thio-, methyl ester C<sub>17</sub>H<sub>23</sub>BrN<sub>2</sub>O<sub>10</sub>S

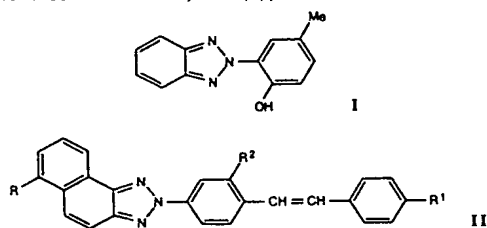
78187-56-1  $\beta$ -D-Glucopyranosiduronic acid, 1,4-dihydro-5-iodo-4-oxo-2-pyrimidinyl 1-thio-, methyl ester C<sub>17</sub>H<sub>23</sub>IO<sub>10</sub>S

78187-57-2  $\alpha$ -L-threo-Hex-4-enopyranosiduronic acid, 1,4-dihydro-4-oxo-2-pyrimidinyl 4-deoxy-1-thio-, methyl ester C<sub>17</sub>H<sub>25</sub>N<sub>2</sub>O<sub>6</sub>S

78187-58-3  $\alpha$ -L-threo-Hex-4-enopyranosiduronic acid, 5-chloro-1,4-dihydro-4-oxo-2-pyrimidinyl 4-deoxy-1-thio-, methyl ester C<sub>17</sub>H<sub>23</sub>ClN<sub>2</sub>O<sub>6</sub>S

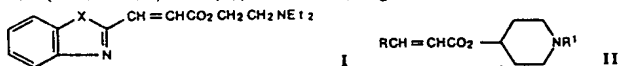
78187-59-4  $\alpha$ -L-threo-Hex-4-enopyranosiduronic acid, 5-bromo-1,4-dihydro-4-oxo-2-pyrimidinyl 4-deoxy-1-thio-, methyl ester C<sub>17</sub>H<sub>23</sub>BrN<sub>2</sub>O<sub>6</sub>S

95: 41674c Mass-spectroscopic study of optical whiteners. V. Mass spectra of derivatives of benzo- and naphthotriazoles. Shibryaeva, L. S.; Ushakova, R. L.; Mikaya, A. I.; Zaikin, V. G. (Nauchno-Issled. Inst. Poluprod. Krasitelei, Moscow, USSR). *Zh. Obshch. Khim.* 1981, 51(2), 447-51 (Russ.). The mass



spectra of I and II [ $R = H, SO_2OPh$ ;  $R^1 = H, Cl$ ;  $R^2 = CN, SO_2OPh, SO_2NH(CH_2)_3NMe_2$ ] indicated that the main fragmentation involved loss of  $N_2H$ . For compds. contg. the  $SO_2OPh$  group, intense peaks corresponding to loss or fragmentation of this group were obsd.

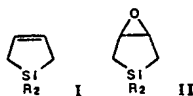
95: 41675d Proton magnetic resonance of some acrylic esters. Ibrahim, E. H. M.; Abdel Rahman, M. O.; Abdellah, I. M. (Fac. Sci., Al-Azhar Univ., Cairo, Egypt). *Egypt. J. Chem.* 1979 (Pub. 1980). 22(4), 265-71 (Eng.). The  $^1H$  NMR of I (X



= O, S) and II ( $R = 2\text{-furyl}$ ,  $R^1 = Me$ ;  $R = 2\text{-benzothiazolyl}$ ,  $R^1 = Et$ ) were obsd. in  $CCl_4$ .

95: 41676e GC/MS analysis of some long chain esters, ketones and propanediol diesters. Vajdi, M.; Nawar, W. W.; Merritt, C., Jr. (Dep. Food Sci. Nutr., Univ. Massachusetts, Amherst, MA 01003 USA). *J. Am. Oil Chem. Soc.* 1981, 58(2), 106-10 (Eng.). In the title study, double hydrogen rearrangement led to the predominant ion in the spectrum of long-chain satd. esters; in the unsatd. esters, a peak corresponding to the loss of alc. from the mol. ion was more pronounced. In contrast to short-chain ketones, McLafferty rearrangement was not the major fragmentation in the spectrum of satd. and unsatd. long-chain ketones.  $\alpha$ -Cleavage was the predominant fragmentation in the spectrum of these ketones. The McLafferty + 1 rearrangement peak was more pronounced for the long-chain ketones than for smaller ketones. Fragmentation patterns of propanediol diesters were similar to those in triglycerides, giving rise to predominant peaks corresponding to acylium ion  $[RCO]^+$  and parent minus acyloxy ion  $[RCOO]^+$ .

95: 41677f Carbon-13 NMR spectra of 1,1-disubstituted 1-sila-3-cyclopentenones and their 3,4-epoxy derivatives. Panasenko, A. A.; Khalilov, L. M.; Tsyrlina, E. M.; Yur'ev, V. P. (Inst. Khim., Ufa, USSR). *Izv. Akad. Nauk SSSR, Ser. Khim.* 1981, (2), 424-7 (Russ.).  $^{13}C$  NMR data were obtained



for I ( $R = Me, Ph, OSiMe_3, OCHMe_2, OMe, OEt, Cl$ ) and II ( $R = Me, Ph, OSiMe_3, OCHMe_2, OCHMe_2, OCHMe_2$ ). The shielding effect of the epoxy ring was manifested in the magnetic nonequivalence of the Me carbons of the  $CHMe_2$  and  $CMe_3$  groups.

95: 41678g Electron impact fragmentation of alkoxy- and thylsilylamines. Piekies, J.; Wojnowski, W.; Meller, A. (Inst. Inorg. Chem. Technol., Tech. Univ., Gdansk, Pol.). *Z. Anorg. Allg. Chem.* 1981, 473, 215-23 (Ger.). The mass spectra of the following compds. were recorded ( $R = Bu, Ph$ ):  $(Me_3CO)_2SiNHR$ ,  $(Me_2CHO)_2SiNHR$ ,  $(Me_2CHO)_2SiMeNHR$ ,  $Me_2CHOSiMe_2NHR$ ,  $Me_3SiNHR$ . The  $N-Bu$  compds. underwent a rearrangement in which H migrated to the silicon center. With the  $N-Ph$  compds. the mol. ion and other radical ions exhibited remarkably high stability. A new rearrangement of the  $NHPh$  group was obsd.

95: 41679h NMR spectroscopic studies of boron compounds. XIX. Carbon-13 NMR studies on monoaminoboranes and borazines. Noeth, Heinrich; Wrackmeyer, Bernd (Inst. Anorg. Chem., Univ. Muenchen, D-8000 Munich, 2 Fed. Rep. Ger.). *Chem. Ber.* 1981, 114(3), 1150-6 (Ger.). Chem. shifts  $\delta(^{13}C)$  of  $R_2BNR_2$  and  $X_2BNR_2$  and of borazines ( $RBNR_2$ ) and ( $XBNR_2$ ) ( $X = halo, OR, SR, NR_2$ ) are related to a  $\gamma$ -effect exerted by R and X on the shielding of  $^{13}C(BC)$  and  $^{13}C(NC)$ . Analogies exist with similar effects in alkenes, immonium salts, and  $C_6H_6$  derivs. Heteronuclear  $^{13}C$  [ $^1H, ^{11}B$ ] triple-resonance expts. permit the observation of sharp  $^{13}C(BC)$  resonance signals.

95: 41680b Reaction of cyclohexanone with ammonium ion under chemical ionization conditions. 1. Formation of protonated unsubstituted imines. Tabet, J. C.; Fraisse, D. (Lab. Synth. Org., Ec. Polytech., 91128 Palaiseau, Fr.). *Org.*

*Mass Spectrom.* 1981, 16(1), 45-7 (Eng.). High resolu. and metastable decompn. spectra were recorded of the ions  $[M + NH_4]^+$  formed by reaction of  $NH_4^+$  with cyclohexanone. The  $m/z$  98 ion, abundant in the  $NH_3$  chem. ionization spectrum of cyclohexanone, is composed of 2 isobaric ions: a protonated imine ion and the mol. ion of cyclohexanone. The former is formed by a process analogous to that which occurs in soln.

95: 41681c The mass spectra of some substituted methyl cinnamates. Zalewski, Romuald I. (Dep. Chem., Univ. Sulaimanyiah, Sulaimanyiah, Iraq). *Org. Mass Spectrom.* 1981, 16(1), 52 (Eng.). The mass spectra were recorded of  $RC_6H_4CH=CHCO_2Me$  ( $R = H, 4-OH, 3-OH, 4-Me, 3-Cl, 4-Cl, 3-Br, 3-NO_2, 4-NO_2$ ). A parent ion of high intensity (40-80%) was present in all spectra and was accompanied by  $[M+1]^+$  and  $[M-1]^+$  peaks. The base peak was in all cases  $[M-31]^+$  (I), formed by loss of  $OMe$ . I loses CO to give the ion  $[M-59]^+$  which decomps. in a typical way for an arom. moiety to give a variety of peaks below  $m/z$  93.

95: 41682d Microwave spectra of dimethyl sulfide- $d_6$ ,  $(CD_3)_2S$ , ground and excited torsional states. Demaison, Jean; Tan, B. T.; Typke, V.; Rudolph, H. D. (Dep. Phys., Univ. Lille I, F-59655 Villeneuve d'Ascq, Fr.). *J. Mol. Spectrosc.* 1981, 86(2), 406-19 (Eng.). The microwave spectra of  $(CD_3)_2S$  in the ground state and 1st and 2nd excited states of Me-top torsion (internal rotation) and of CSC deformation as well as the ground-state spectra of the  $^{13}C$ - and  $^{34}S$ -substituted forms were measured. The rotational consts. and centrifugal-distortion and rotation-vibration interaction consts. were detd. The rotational lines in the excited torsional states (1, 1, 2, 2, 2, 2) were split into quartets, owing to the interaction between mol. rotation and Me-top internal rotation. The exptl. multiplet splittings were fitted to those calcd. from a rotation-internal rotation Hamiltonian in order to obtain values for the internal-rotation barrier  $V_3$  and the top-top interaction potential coeffs.  $V_{12}$  and  $V_{12}^2$ ;  $V_{12}$  was too highly correlated with  $V_3$  for a sep. detn. The values following from the least-squares adjustment are discussed.

95: 41683e Acetic acid: microwave spectra, internal rotation and substitution structure. Van Eijk, B. P.; Van Opheusden, J.; Van Schaik, M. M. M.; Van Zoeren, E. (Dep. Struct. Chem., Univ. Utrecht, 3584 CH Utrecht, Neth.). *J. Mol. Spectrosc.* 1981, 86(2), 465-79 (Eng.). The internal-rotation splittings in the microwave spectrum of AcOH were reexamd., using both principal-axis method (PAM) and internal-axis method (IAM) treatments. Individual terms in the PAM equation correlated with the 1st terms in an expansion of the corresponding IAM formula. When centrifugal distortion was allowed for, both methods reproduced the A-type frequencies within exptl. error. To derive the substitution structure, 8 isotopic species were studied. The inertial moments of the mols. with various degrees of Me-group deuteration are not consistent with each other, so these data could not be fully used. Therefore, the structure was derived with the assumption of a cylindrically sym. Me group, although there is some evidence that the HCH angles differ by a few degrees. The geometry, which agrees with earlier electron-diffraction results, is compared with the substitution structures of other carboxylic acids.

95: 41684f Refinements of mass spectrometry/mass spectrometry and applications to organic analysis. Sigsby, Mary Lou (Purdue Univ., West Lafayette, IN USA). 1980. 226 pp. (Eng.). Avail. Univ. Microfilms Int., Order No. 8102708. From *Diss. Abstr. Int. B* 1981, 41(8), 3022.

95: 41685g Spectral characteristics of drugs with an oxygen heteroatom. Buryak, V. P. (Med. Inst., Zaporozhe, USSR). *Farm. Zh. (Kiev)* 1981, (1), 68-9 (Ukrain.). The UV spectrum of khellin has absorption max. at 242-51, 280-4 and 320-37 nm, the last one being the most characteristic of furochromone systems and corresponding to a  $\pi \rightarrow \pi^*$  transition.

95: 41686h  $C_3H_3^+$  in flames and the proton affinity of cyclopropenylidene or propadienylidene ( $C_3H_2$ ). McAllister, Trevor; Nicholson, Anthony J. C. (Div. Chem. Phys., CSIRO, Clayton, 3168 Australia). *J. Chem. Soc., Faraday Trans. 1* 1981, 77(4), 821-5 (Eng.).  $C_3H_3^+$  was prominent in the reaction zone of a  $CH_4 + Ar$  flame, but was displaced by  $NH_4^+$  when  $NH_3$  was added. These observations were explained in terms of the equil. in the proton-transfer reactions  $H_3O^+ + C_3H_2 \rightleftharpoons C_3H_3^+ + H_2O$  (A) and  $NH_4^+ + C_3H_2 \rightleftharpoons C_3H_3^+ + NH_3$  (B). In reaction A, the proton affinity of  $C_3H_2$  is much greater than that of  $H_2O$ , leading to  $H_3O^+$  formation in substantial amts. only when the  $H_2O$  concn. is several orders of magnitude larger than that of  $C_3H_2$ . In reaction B, the higher proton affinity of  $NH_3$  ensures that  $NH_4^+$  dominates the reaction zone. Ion-cyclotron-resonance expts. showed that the proton affinity of  $C_3H_2$  is  $>65$  kJ/mol greater than that of  $NH_3$ . The concn. of  $C_3H_2$  in the reaction zone was estd. as  $7 \times 10^{12}$  cm $^{-3}$  lower than the detection limit of mass spectrometry.

95: 41687j Fast searching for identical carbon-13 NMR spectra via inverted files. Bremser, W.; Wagner, H.; Franke, B. (Cent. Res., BASF A.-G., D-6700 Ludwigshafen, Fed. Rep. Ger.). *Org. Magn. Reson.* 1981, 15(2), 178-87 (Eng.). For large mols. and incomplete spectra, computer matching of